

Study of couplings effect on the performance of a spin-current diode: Nonequilibrium Green's function based model

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Abstract

In this paper, spin-dependent transport through a spin diode composed of a quantum dot coupled to a normal metal and a ferromagnetic lead is studied. The current polarization and the spin accumulation are analyzed using the equations of motion method within the nonequilibrium Green's function formalism. We present a suitable method for computing the Green's function without carrying out any self-consistent calculation. Influence of coupling strength and magnetic field on the spin current is studied and observed that this device can not work as a spin diode under certain conditions.

1 Introduction

Spin-dependent transport through a quantum dot (QD) has attracted increasing attention in recent years due to development in constructing spin-based devices [1, 2, 3, 4, 5]. Study of transport through QDs obtains interesting information about novel physics phenomena such as Kondo effect [6, 7, 8], spin and Coulomb blockade effects [9, 10, 11, 12], spin valve effect [13, 14], tunneling magnetoresistance [15, 16], zero-bias anomaly [17] and etc. Coupling the QD to the different contacts can lead to form different devices for example the spin filters constructed by coupling the QD to the normal metals [18, 19] and spin diodes constructed by attaching the QD to a normal metal and a ferromagnetic lead [20].

Recently, spin diodes have been studied both experimentally and theoretically. C. A. Merchant and N. Marković [20] observed diode-like behavior in a carbon nanotube coupled to a ferromagnetic and a nonmagnetic lead. The spin diode-like behavior was also reported by Ivan and co-workers [21] in resonant tunneling sandwiched by tunnel barriers with different spin-dependent transparencies. In addition, spin diode devices were theoretically analyzed in a few articles. Souza and co-workers [22] studied a semiconductor QD coupled to a

normal metal and a ferromagnetic metal and I. Weymann and co-workers [23] studied a spin diode composed of a carbon nanotube coupled to a normal metal and a ferromagnetic metal. Both of them used rate equations [24, 25] which are valid in the limit $\Gamma_0 \ll kT$ that Γ_0 and T are coupling strength and temperature, respectively. Here, we use the nonequilibrium Green's function formalism (NEGF) [26] also valid in the limit $\Gamma_0 \gtrsim kT$ to analyze spin diode behavior composed of a quantum dot. The Green's function is obtained by means of the equations of motion method within the nonequilibrium Green's function formalism up to the second order of Hartree-Fock approximation [27]. We extract an analytical relation for the electron density without performing any self-consistent calculation. The obtained result can be useful for studying charge transport through mesoscopic systems by means of equations of motion method within Green's function formalism. The influence of spin splitting on the performance of the device is investigated. This splitting can be created by an external magnetic field or coupling of the dot to a magnetic substrate. In addition, the influence of coupling strength on the diode behavior is analyzed. Such an examination is impossible by means of the rate equations because it is just valid in the limit of very weak coupling.

The article is organized as follows: the model Hamiltonian and main formulas are presented in section 2, in section 3 we present numerical results and discuss the difference between results obtained from NEGF and rate equations. In the end, some sentences are given as a conclusion.

2 Description of the model

Hamiltonian describing a quantum dot coupled to a ferromagnetic and a non-magnetic lead is written as

$$H = \sum_{\alpha,k,\sigma} \varepsilon_{\alpha,k,\sigma} c_{\alpha,k,\sigma}^\dagger c_{\alpha,k,\sigma} + \sum_{\sigma} \varepsilon_{\sigma} n_{\sigma} + U n_{\uparrow} n_{\downarrow} + \sum_{\alpha,k,\sigma} [T_{\alpha,k,\sigma} c_{\alpha,k,\sigma}^\dagger d_{\sigma} + T_{\alpha,k,\sigma}^\dagger d_{\sigma}^\dagger c_{\alpha,k,\sigma}] \quad (1)$$

where $c_{\alpha,k,\sigma}^\dagger (c_{\alpha,k,\sigma})$ creates (annihilates) an electron with momentum k , spin σ in the lead α . $\varepsilon_{\sigma} = \varepsilon_0 + \sigma\Delta$ is the energy level of the dot, $\Delta = 2g\mu_B B$ denotes Zeeman splitting, B is magnetic field and σ is equal to 1(-1) for $\uparrow(\downarrow)$, respectively. $d_{\sigma}^\dagger (d_{\sigma})$ is the creation (annihilation) operator in the dot and $n_{\sigma} = d_{\sigma}^\dagger d_{\sigma}$ is the occupation operator. U is on-site Coulomb interaction strength, $T_{\alpha,k,\sigma}$ describes tunneling between the dot and the lead α and it is also assumed that the electron spin is conserved during the tunneling.

In order to analyze the system, the nonequilibrium Green's function method has been used. The retarded Green's function of the dot is $G_{\sigma}^r = -i\Theta(t-t') < \{d_{\sigma}(t), d_{\sigma}^\dagger(t')\} >$ that in the steady state it only depends on the time difference $\tau = t-t'$. Hence, it is better to use its Fourier transform $G_{\sigma}^r(\epsilon) = < < d_{\sigma}, d_{\sigma}^\dagger > >_{\epsilon}$. Using the equations of motion technique for the nonequilibrium Green's func-

tion up to the second Hartree-Fock approximation, the spin-dependent Green's function of the dot is given by

$$G_{\sigma}^r(\epsilon) = \frac{1 - \langle n_{\bar{\sigma}} \rangle}{\epsilon - \varepsilon_{\sigma} + \frac{i}{2}(\Gamma_{\sigma}^L(\epsilon) + \Gamma_{\sigma}^R(\epsilon))} + \frac{\langle n_{\bar{\sigma}} \rangle}{\epsilon - \varepsilon_{\sigma} - U + \frac{i}{2}(\Gamma_{\sigma}^L(\epsilon) + \Gamma_{\sigma}^R(\epsilon))} \quad (2)$$

where $\Gamma_{\sigma}^{\alpha}(\epsilon) = 2\pi \sum_k |T_{\alpha,k,\sigma}|^2 \delta(\epsilon - \varepsilon_{\alpha,k,\sigma})$ is the coupling strength giving rise to the broadening of the dot levels due to tunneling through the left and right leads and $\bar{\sigma}$ stands for the opposite spin σ . In the following we use the wide band limit i.e. the energy independent broadening $\Gamma_{\sigma}^{\alpha}(\epsilon) = \Gamma_{\sigma}^{\alpha}$. The electron density is given by [27]

$$\langle n_{\sigma} \rangle = -2 \int \frac{d\epsilon}{2\pi} \frac{f^L(\epsilon)\Gamma_{\sigma}^L + f^R(\epsilon)\Gamma_{\sigma}^R}{\Gamma_{\sigma}^L + \Gamma_{\sigma}^R} \text{Im}(G_{\sigma}^r(\epsilon)) \quad (3)$$

that $f^{\alpha}(\epsilon)$ denotes the Fermi distribution function of the lead α with the chemical potential μ_{α} . Although it seems Eqs.(2,3) should be solved in a self-consistent manner to obtain the exact Green's function, we show the Green's function and the electron density can be analytically computed. From Eq.(2) the retarded Green's function can be written as follows [28]

$$G_{\sigma}^r(\epsilon) = A_{\sigma}(\epsilon) + B_{\sigma}(\epsilon) \langle n_{\bar{\sigma}} \rangle \quad (4)$$

where

$$A_{\sigma}(\epsilon) = \frac{1}{\epsilon - \varepsilon_{\sigma} + \frac{i}{2}(\Gamma_{\sigma}^L + \Gamma_{\sigma}^R)} \quad (5a)$$

$$B_{\sigma}(\epsilon) = \frac{U}{(\epsilon - \varepsilon_{\sigma} + \frac{i}{2}(\sum_{\alpha} \Gamma_{\sigma}^{\alpha}))(\epsilon - \varepsilon_{\sigma} - U + \frac{i}{2}(\sum_{\alpha} \Gamma_{\sigma}^{\alpha}))} \quad (5b)$$

If Eq.(4) is substituted into Eq.(3), it can be easily shown that the spin-dependent density is given by

$$\langle n_{\sigma} \rangle = \frac{Q_{\sigma} + R_{\sigma}Q_{\bar{\sigma}}}{1 - R_{\sigma}R_{\bar{\sigma}}} \quad (6)$$

where

$$Q_{\sigma} = -2 \int \frac{d\epsilon}{2\pi} \frac{\Gamma_{\sigma}^L f^L(\epsilon) + \Gamma_{\sigma}^R f^R(\epsilon)}{\Gamma_{\sigma}^L + \Gamma_{\sigma}^R} \text{Im}(A_{\sigma}(\epsilon)) \quad (7a)$$

$$R_{\sigma} = -2 \int \frac{d\epsilon}{2\pi} \frac{\Gamma_{\sigma}^L f^L(\epsilon) + \Gamma_{\sigma}^R f^R(\epsilon)}{\Gamma_{\sigma}^L + \Gamma_{\sigma}^R} \text{Im}(B_{\sigma}(\epsilon)) \quad (7b)$$

Knowing the electron density Eq.(6), the Green's function is obtained from Eq.(4). Now, we are able to compute the current given by ($e = \hbar = 1$) [29]

$$I_{\sigma} = -2 \int \frac{d\epsilon}{2\pi} [f^L(\epsilon) - f^R(\epsilon)] \frac{\Gamma_{\sigma}^L \Gamma_{\sigma}^R}{\Gamma_{\sigma}^L + \Gamma_{\sigma}^R} \text{Im}(G_{\sigma}^r(\epsilon)) \quad (8)$$

For simulation purpose, we set $U = 4meV$, $kT = 212meV$ which is large enough to guarantee no Kondo effect and $\varepsilon_\sigma = 1meV + \sigma\Delta$ that Δ is equal to $1.16 \times 10^{-4}meV$ or $0.174meV$ for $B = 10^{-3}T$ and $1.5T$, respectively. The coupling strength for the metal lead is set $\Gamma_\uparrow = \Gamma_\downarrow = \Gamma_0$ and for ferromagnetic lead $\Gamma_{\uparrow(\downarrow)} = \Gamma_0(1 \pm p)$ that p stands for the spin polarization degree of the lead. The chemical potential of the left lead (normal metal) is equal to zero and for right one, we set $\mu^R = -V$, so when the bias is positive the left lead acts as an emitter and in the negative bias it acts as a collector.

3 Simulation results

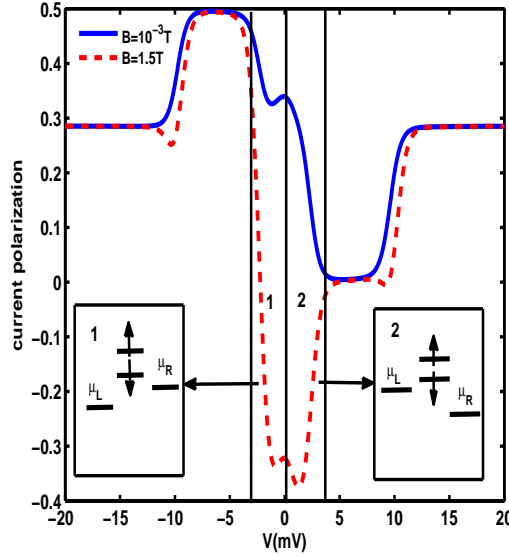


Figure 1: The current polarization as a function of bias in weak magnetic field (solid) and strong magnetic field (dashed). The parameters are $p = 0.5$ and $\Gamma_0 = 30\mu eV$. The left and right insets show the QD levels and the chemical potentials of the leads in the regions 1 and 2, respectively. Energy difference between \uparrow and \downarrow levels depends on the magnitude of the magnetic field.

Fig. 1 shows the current polarization $\xi = \frac{I_\uparrow - I_\downarrow}{I_\uparrow + I_\downarrow}$ as a function of the bias voltage in different magnetic fields. It is observed that in positive bias when $\mu^R < \varepsilon_\sigma$ and $\varepsilon_\sigma < \mu^L < \varepsilon_\sigma + U$ (the dot is singly occupied) the current polarization becomes zero because in positive bias the normal metal lead acts as an emitter and the spin-up current is equal to spin-down current due to $\Gamma_\uparrow^L = \Gamma_\downarrow^L$. Note that when the QD is singly occupied, the current polarization

depends on $(\Gamma_{\uparrow}^{\alpha} - \Gamma_{\downarrow}^{\alpha})$ that α denotes the emitter lead [22]. In negative bias, the ferromagnetic lead acts as an emitter and the current polarization becomes maximum when $\varepsilon_{\sigma} < \mu^R < \varepsilon_{\sigma} + U$ because of $\Gamma_{\uparrow}^R > \Gamma_{\downarrow}^R$ so that the spin-up current is bigger than the spin-down current. This behavior suggests that this system operates as a spin diode in a definite voltage range. We also observe the current polarization behaves completely different in the response to weak and strong magnetic fields in the regions 1 and 2 shown in the fig. 1. Although our results and the results given in [22] are nearly the same in weak B and Γ_0 , they are completely different in strong field because of removing degeneracy [30]. The left inset can help us to understand the current polarization behavior in the region 1 where the ferromagnetic lead acts as the emitter and the dot levels are outside the bias window. In the weak magnetic field ($B = 10^{-3}T$) ε_{\uparrow} and ε_{\downarrow} are nearly degenerate so that the spin-up can be occupied faster than the other spin due to $\Gamma_{\uparrow}^R > \Gamma_{\downarrow}^R$ and as a result $I_{\uparrow} > I_{\downarrow}$, therefore, ξ is positive. In the strong magnetic field ($B = 1.5T$), the levels of the spin-up and spin-down are split so that the ε_{\downarrow} is more energetically accessible hence $I_{\downarrow} > I_{\uparrow}$ and as a result the current polarization becomes negative. The right inset describes the position of the chemical potentials of the leads and the energy levels of the dot in the region 2 in which the normal metal lead acts as the emitter. In weak magnetic field both levels have the same energy the \uparrow electron can leave the dot faster due to $\Gamma_{\uparrow}^R > \Gamma_{\downarrow}^R$ therefore I_{\uparrow} is bigger than I_{\downarrow} and the current polarization is positive, But in the strong magnetic field the \downarrow electron state is occupied faster because it is more accessible and as a consequence, $I_{\downarrow} > I_{\uparrow}$ so that the current polarization becomes negative. When $|V| > \varepsilon_{\sigma} + U$ that the dot is doubly occupied the current polarization will be constant due to interplay between the spin accumulation and the electron-electron interaction.

Fig. 2 plots the spin current $I_{spin} = I_{\uparrow} - I_{\downarrow}$ versus the bias voltage for different coupling strengths. As we expect with increase of Γ_0 the current is enhanced because of faster tunneling. We observe when $|\varepsilon_{\sigma}| < |eV| < |\varepsilon_{\sigma} + U|$, the spin current as well as the current polarization becomes zero just in the limit of low or intermediate Γ_0 and with increasing the coupling strength the current polarization deviates from zero and as a result the device can not work as a spin diode. The dependence of the spin current on Γ_0 is shown in the inset in the conditions that the dot is singly occupied. It is observed that NEGF and rate equation obtain the same result for $\Gamma_0 < 0.05meV$, but the latter one could not describe the system well for $\Gamma_0 > 0.05meV$. Indeed, the rate equation predicts $\xi = 0$ for any value of Γ_0 . The unexpected positive and negative spin current has been also observed in the regions 1 and 2, respectively. Note that the current is measured from the left lead i.e. the current is positive in the positive bias. The positive spin current in the region 1 means that I_{\downarrow} is bigger than I_{\uparrow} because of $\varepsilon_{\downarrow} < \varepsilon_{\uparrow}$. The negative spin current in the region 2 shows that $I_{\downarrow} > I_{\uparrow}$ due to the same reason.

Fig. 3 shows the spin accumulation $m = n_{\uparrow} - n_{\downarrow}$ as a function of the bias voltage. It is observed that in the negative bias the spin accumulation is positive because in this situation the right lead acts as the emitter and the \uparrow electron is injected faster and hence the spin-up population is more. In negative bias that

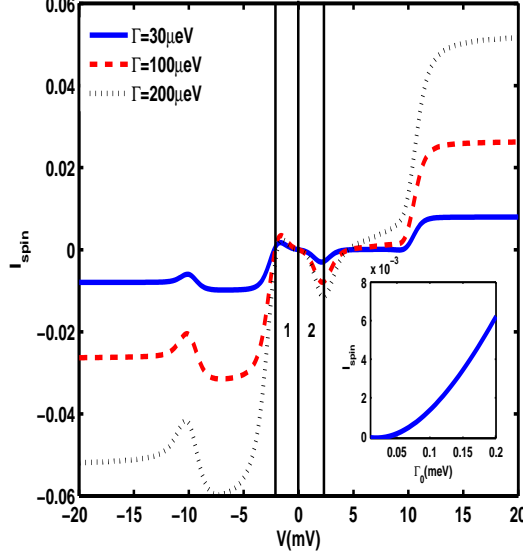


Figure 2: The spin current versus bias in different Γ_0 . We set $B = 1.5T$. Inset shows variation of the spin current as function of broadening in $V = 9mV$.

the right lead acts as the collector, the spin accumulation is negative because a \downarrow electron has to stay inside the dot for a longer time. Such a behavior was recently reported using the rate equations method. Here, there is a significant difference between the results presented in the Ref [22] and our results obtained using the Green's function method. In $p = 1$ that the right lead is a half metal and in the positive bias when the energy level of the dot is inside the bias window, the spin accumulation is equal to -1 (the gray line in the fig. 3b) in the weak broadening ($\Gamma_0 = 10\mu eV$). Indeed, the \downarrow electron injected from the left lead can not leave the dot and since the second level $\varepsilon_\sigma + U$ is outside the bias window, the dot contains only a \downarrow electron. But in the other case $\Gamma_0 = 200\mu eV$, we observe the spin accumulation is about -0.8. This difference originates due to different density of states (DOS) in these couplings. In the weak coupling (fig. 3c) the DOS of the \uparrow electron has a peak outside the bias window but the peak of the DOS of the \downarrow electron is inside the bias window and as a result the \downarrow electron only exists inside the dot. In the strong coupling (fig. 3d) the DOS is broadened and the DOS of the \uparrow electron has a peak inside the bias window therefore the fraction of the \uparrow electron can exist inside the dot leading to the decrease of the spin accumulation.

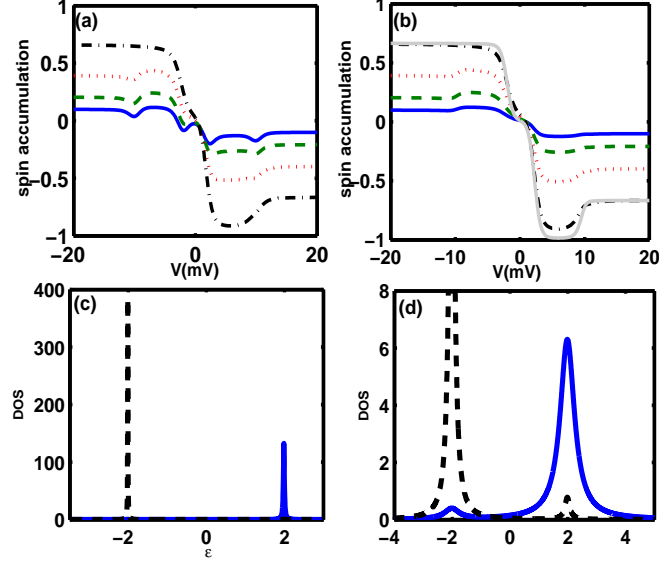


Figure 3: The spin accumulation as a function of polarization in (a) strong magnetic field and (b) weak magnetic field. We set $p = 0.2$ (solid), $p = 0.4$ (dashed), $p = 0.7$ (dotted) and $p = 1$ (dash-dotted). $\Gamma_0 = 200 \mu\text{eV}$ in all plots except the gray line in (b) equal to $10 \mu\text{eV}$. (c) and (d) show DOS (spin-down (dashed) and spin-up (solid)) in weak and strong couplings, respectively.

4 Conclusion

In this paper, spin-dependent transport through a quantum dot attached to a normal metal and a ferromagnetic lead is studied by using the nonequilibrium Green's function formalism. We examine under what conditions this device can work as a spin diode. We also investigate the influence of magnetic field on the current polarization. It is observed that coupling strength has an important role in the performance of the device. More specifically, in the strong coupling this device can not work properly. It is also observed when the dot is coupled to a half metal lead, the spin accumulation is equal to -1 in the weak coupling but it deviates from -1 in the strong coupling.

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